On The Validity Domain of the First Born Approximation in X-ray Diffraction Microscopy

David Shapiro¹, Chris Jacobsen², Edwin Widjonarko³

¹Lawrence Berkeley National Laboratory, ²Stony Brook University, ³University of California at Berkeley

We are investigating the validity domain of the first Born approximation as applied to coherent x-ray diffraction microscopy. We simulate the x-ray diffraction patterns of objects of varying size and composition by multi-slice propagation of a plane x-ray wavefield through the object followed by a Fourier transform. We then reconstruct the object using the RASR algorithm both with and without applying a reality constraint. We find that the convergence error rises steadily with object thickness when a reality constraint is applied while it remains reasonably flat without the constraint. Furthermore, we have identified a thickness threshold, above which, the reconstruction algorithm is no longer capable of solving asymmetric structures when a reality constraint is applied. This threshold is plotted as a function of material density and x-ray wavelength. It is interpreted to be the point at which the far-field diffraction pattern becomes so significantly asymmetric that it can be assumed to not satisfy the first Born approximation and may serve as an upper bound on its validity. In fact, the complex values of the exit wavefield, which are used to generate the diffraction patterns, fit nicely within the first Rytov approximation. We discuss the implications of these results for experimenters wishing to do three-dimensional reconstructions from a tilt series of two-dimensional diffraction patterns.